

# Searches for violation of fundamental time reversal and space reflection symmetries in solid state experiments

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The electric dipole moment (EDM) of a particle violates both time reversal (T) and space reflection (P) symmetries. There have been recent suggestions for searches of the electron EDM using solid state experiments [1,2]. These experiments could improve the sensitivity compared to present atomic and molecular experiments by several orders of magnitude. In the present paper we calculate the expected effect. We also suggest that this kind of experiment is sensitive to T,P-violation in nuclear forces and calculate effects caused by the nuclear Schiff moment.

The compounds under consideration contain magnetic  $Gd^{3+}$  ions and oxygen  $O^{2-}$  ions. We demonstrate that the main mechanism for the T,P-odd effects is related to the penetration of the Oxygen 2p-electrons to the Gd core. All the effects are related to the deformation of the crystal lattice.

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## I. INTRODUCTION

Violation of the combined symmetry of charge conjugation (C) and parity (P) has been discovered in the decay of the  $K^0$  meson about 40 years ago [3]. The exact origin of this symmetry violation remains an enigma, although the so called standard model of electroweak interactions can describe these processes phenomenologically. It has also been proposed by Sakharov [4] that the matter-antimatter asymmetry observed in our Universe could have arisen from a CP-violating interaction active at an early stage of the Big Bang. The CP-violation implies a time-reversal (T) asymmetry and hence violation of both T- and P-symmetries, because there are strong reasons to believe that the combined CPT-symmetry should not be violated [5]. Electric dipole moment (EDM) of a system in a stationary quantum state indicates violation of T- and P-symmetries. This is why searches for EDM of elementary particles, atoms and molecules are very important for studies of violations of fundamental symmetries [6]. A property that is closely related to EDM is the so called Schiff moment, see e.g. Ref. [6]. A non zero Schiff moment also indicates T- and P-violation. In the present paper we consider T,P-odd effects in solids due to the EDM of the electron and due to the nuclear Schiff moment.

The present best limitation on the electron EDM comes from the Berkeley experiment with an atomic Thallium beam [7],

$$d_e < 1.6 \times 10^{-27} e \text{ cm}. \quad (1)$$

There are some ideas for improvement of the sensitivity. One way of improvement is an experiment with metastable levels of PbO molecules [8]. A breakthrough could be achieved in solid state experiments with compounds containing uncompensated spins. This idea was suggested by Shapiro in 1968 [9]. Application of a strong electric field to electrons bound within a solid would align the EDMs of these electrons. This should lead to a simultaneous alignment of the electron spins; the magnetic field arising from this alignment could be detected experimentally. Another possibility is to polarize electrons by the external magnetic field. This causes alignment of electron EDMs, and hence induces a voltage across the sample that could be detected. An experiment of this kind has been performed with nickel-zinc ferrite [10]. However due to experimental limitations the result was not very impressive. Interest in this approach has been renewed recently due to a suggestion of Lamoreaux [1] and Hunter [2] to perform similar experiments with Gadolinium Gallium Garnet,  $Gd_3Ga_5O_{12}$  (GGG), and Gadolinium Iron Garnet  $Gd_3Fe_5O_{12}$  (GdIG) employing new experimental techniques. The estimates of sensitivity look highly promising. In the present work we calculate the expected effects.

The best limitation on the Nuclear Schiff moment (NSM) comes from the Seattle experiment with atomic  $^{199}\text{Hg}$  [11],

$$S_N(^{199}\text{Hg}) < 0.7 \times 10^{-49} e \text{ cm}^3. \quad (2)$$

The expected value of  $S_N$  expressed in terms of the fundamental CP-violating interaction depends on the structure of the particular nucleus, however for heavy nuclei this dependence is not that strong and therefore we will take the value (2) as a reference point. Later, we will comment on a possible additional enhancement due to a special structure of the  $^{155}\text{Gd}$  nucleus. One can search for NSM in the experiments with GGG and GdIG simultaneously with searches for the electron EDM. The point is that due to the hyperfine interaction

nuclear polarization causes polarization of electrons and vice versa. Another possibility is to use a compound without unpaired electrons, for example Lutetium Gallium Garnet,  $\text{Lu}_3\text{Ga}_5\text{O}_{12}$  or Lutetium Oxide  $\text{Lu}_2\text{O}_3$ . In this case one can cool the nuclear spin subsystem down to very low temperature [12] and this gives an additional enhancement of the effect. In the present work we calculate the coefficient of proportionality between voltage and nuclear polarization due to NSM.

Structure of the paper is the following. In Section II we present simple estimates of the effects induced by the electron EDM. Section III contains derivation of the effective interaction induced by the electron EDM. The  $\text{Gd}^{3+}$  octupole moment is also discussed here. In Section IV we calculate wave functions of Oxygen electrons penetrating inside the  $\text{Gd}^{3+}$  core. Section V presents derivation of the effective Hamiltonian which relates the electron EDM with deformation of the lattice. In Sections VI and VII we derive final results for the voltage across the sample and the energy shift in the external electric field induced by the electron EDM. Section VIII presents similar results for effects induced by the Gd Nuclear Schiff Moment. Finally Sections IX and X contain estimates of accuracy of the calculations and our conclusions.

## II. SIMPLE ESTIMATES FOR EFFECTS RELATED TO THE ELECTRON EDM

In this section we follow simple and important estimates performed in Ref. [1]. GdIG is an ionic crystal consisting of  $\text{Gd}^{3+}$ ,  $\text{Fe}^{3+}$  and  $\text{O}^{2-}$  ions, see Ref. [13]. Uncompensated electronic spins are localized at  $\text{Gd}^{3+}$  which has a  $4f^7$  electronic configuration and  $\text{Fe}^{3+}$  which has a  $4d^5$  electronic configuration. Both these ions have half-filled electronic shells, hence the orbital angular momenta of these shells are zero. This explains a very weak spin anisotropy in this compound. If the electron EDM is not zero, then both  $\text{Gd}^{3+}$  and  $\text{Fe}^{3+}$  have induced EDMs proportional to  $d_e$ ,  $d_a = Kd_e$ . It is known that the coefficient  $K$  scales as  $Z^3$ , where  $Z$  is the nuclear charge, see, e.g. [6]. Therefore we neglect the EDM of  $\text{Fe}^{3+}$  and consider only  $\text{Gd}^{3+}$ . GGG differs from GdIG in the replacement of magnetic  $\text{Fe}^{3+}$  by nonmagnetic  $\text{Ga}^{3+}$  ions. The most important  $\text{Gd}^{3+}$  ion is exactly the same. The enhancement coefficient for  $\text{Gd}^{3+}$  has been calculated previously [14]

$$d_a = Kd_e, \quad K = -4.9 \pm 1.6 \quad (3)$$

If all the uncompensated spins in the sample are 100% polarized then the induced electric field in the sample is  $E = 4\pi n_{\text{Gd}} d_a$ , where  $n_{\text{Gd}} = 1.235 \times 10^{22} \text{cm}^{-3}$  is the number density of Gd. This gives the following induced voltage across an  $L = 10 \text{cm}$  sample

$$V = EL = 4\pi n_{\text{Gd}} K d_e L = 2 \times 10^{-9} V. \quad (4)$$

This numerical estimate corresponds to the current limitation on  $d_e$ , see (1) and would be absolutely correct for a crystal consisting of neutral atoms or molecules. However the charge of  $\text{Gd}^{3+}$  is not zero. Hence the average electric field acting on the ion must be equal to zero, and hence the EDM of the ion cannot really produce the field (4). This means that the crystal lattice relaxes in such a way that the effect (4) is canceled out. This is the Schiff theorem [15]. The theorem is violated due to the finite size of the ion. It means that the estimate (4) should be reduced by some factor depending on the ratio of the ion size to the lattice spacing. Calculation of this effect is performed in the following sections.

One can also perform an estimate of the resulting magnetization due to an applied electric field  $E_0$  to the sample. The field inside the solid is  $E = E_0/\epsilon$  where  $\epsilon$  is the dielectric constant (for GdIG  $\epsilon \approx 15$ , and for GGG  $\epsilon \approx 30$  see Ref. [16]) The T,P-odd energy shift per Gd ion is given by,

$$\delta\epsilon = d_a E = K d_e E = 0.9 \times 10^{-22} eV. \quad (5)$$

The numerical estimate corresponds to the current limitation on  $d_e$ , see (1) and  $E = 10 \text{kV/cm}$ . Using Boltzmann distribution one can deduce the resulting magnetization of the medium. Similar to (4) the estimate (5) contradicts the Schiff theorem. An accurate calculation of  $\delta\epsilon$  is performed below.

## III. INTERACTION OF THE $\text{GD}^{3+}$ ION WITH ENVIRONMENT, VANISHING OF THE OCTUPOLE MOMENT OF THE ION

In this section we follow the method of calculation suggested in Ref. [17] (see also [6]). Let

$$\phi(\mathbf{r}) = \int d^3R \frac{eq(\mathbf{R})}{|\mathbf{r} - \mathbf{R}|} - \mathbf{r} \cdot \mathbf{E}_{ext} \quad (6)$$

be the electric potential produced by the environment of a particular  $\text{Gd}^{3+}$  ion,  $q(\mathbf{R})$  is the charge density of surrounding ions and  $\mathbf{E}_{ext}$  is the electric field produced by distant ions and external sources.

The energy correction for a system which has a non-zero EDM is

$$\Delta\epsilon = e \int d^3r \delta\rho(\mathbf{r})\phi(\mathbf{r}). \quad (7)$$

where  $\delta\rho(\mathbf{r})$  is the correction to the charge density of  $\text{Gd}^{3+}$  due to the T,P-odd interaction  $H_{TP}$ .

In equilibrium the average force acting on  $\text{Gd}^{3+}$  vanishes,

$$\langle F_{Gd^{3+}} \rangle = -e \int d^3r \rho_0 \nabla_r \phi(\mathbf{r}) = 0. \quad (8)$$

Here  $\rho_0(\mathbf{r})$  is the spherically symmetric charge density of  $\text{Gd}^{3+}$  normalized by the condition  $\int d^3r \rho_0(\mathbf{r}) = 3$ . The total charge density of  $\text{Gd}^{3+}$  is given by  $\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \delta\rho(\mathbf{r})$ .

Using eqs. (7) and (8) and assuming that  $\mathbf{E}_{ext}$  is uniform in the vicinity of  $\text{Gd}^{3+}$  one can rewrite the energy correction as

$$\begin{aligned} \Delta\epsilon &= e \int d^3r \delta\rho(\mathbf{r})\phi(\mathbf{r}) - \frac{1}{3} \int d^3r \rho_0(\mathbf{r})(\mathbf{d}_a \cdot \nabla_r)\phi(\mathbf{r}) \\ &= e^2 \int d^3R q(\mathbf{R}) \int d^3r \left( \frac{\delta\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{R}|} + \frac{1}{3}(\mathbf{d}_a \cdot \nabla_R) \frac{\rho_0(\mathbf{r})}{|\mathbf{r} - \mathbf{R}|} \right). \end{aligned} \quad (9)$$

The charge density correction  $\delta\rho(\mathbf{r})$  can be expanded in a series of spherical harmonics,

$$\delta\rho(\mathbf{r}) = \sum_{lm} f_{lm}(r) Y_{lm}(\theta_r, \phi_r), \quad (10)$$

where

$$f_{lm}(R) \propto \sum_n \frac{\langle 0 | \delta(R-r) Y_{lm} | n \rangle \langle n | H_{TP} | 0 \rangle}{E_0 - E_n}. \quad (11)$$

Here we denote the argument of  $f_{lm}$  by  $R$  to distinguish it from the internal variable  $r$  in the matrix elements. Because of the negative parity of  $H_{TP}$  only odd  $l$  contribute to (10). The  $Y_{1m}$  terms correspond to the EDM of  $\text{Gd}^{3+}$ , and  $Y_{3m}$  to its octupole moment. First we demonstrate that the octupole and all higher moments vanish for  $\text{Gd}^{3+}$  if one neglects the spin-orbit interaction. The kinematic structure of the T,P-odd Hamiltonian is, see, e.g. [6]

$$H_{TP} = a(r) \mathbf{s} \cdot \mathbf{n}_r, \quad (12)$$

where  $\mathbf{s}$  and  $\mathbf{r}$  are the spin and the position of the electron, and  $\mathbf{n}_r = \mathbf{r}/r$ . An intermediate state  $|n\rangle$  in (11) belongs to some electronic configuration. We denote the configuration by  $\bar{n}$ . The states within the configuration we numerate by an index  $\alpha$ , so  $|n\rangle = |\bar{n}_\alpha\rangle$ . We also denote by  $E_{\bar{n}}$  the average energy of the configuration. In eq.(11) we first perform summation over  $\alpha$  and then over  $\bar{n}$ . With account of (12) this gives

$$f_{lm}(R) \propto \sum_{\bar{n}} \frac{\langle 0 | \delta(R-r) | \bar{n} \rangle \langle \bar{n} | a(r) | 0 \rangle}{E_0 - E_{\bar{n}}} \langle 0 | Y_{lm} s_i n_i | 0 \rangle \quad (13)$$

Here we have used the closure relation  $\sum_\alpha |\bar{n}_\alpha\rangle \langle \bar{n}_\alpha| = 1$ , where 1 acts in the spin-angular space. This relation is valid because of the separation of variables in the problem. Without the spin-orbit interaction, the ground state of  $\text{Gd}^{3+}$  reads

$$|0\rangle = |L=0\rangle |S=7/2\rangle, \quad (14)$$

where  $|L=0\rangle$  is the S-wave orbital state (half filled shell). Hence we get from (13)

$$f_{lm} \propto \langle 0 | Y_{lm} s_i n_i | 0 \rangle = \langle L=0 | Y_{lm} n_i | L=0 \rangle \langle S=7/2 | s_i | S=7/2 \rangle. \quad (15)$$

It is clear that this equation gives zero for any  $l$  higher than 1 because one can combine  $Y_{lm}$  with  $\mathbf{n}$  into total angular momentum zero only at  $l=1$ . The spin-orbit interaction  $\mathbf{l} \cdot \mathbf{s}$  admixes states with nonzero  $L$  to the ground state of  $\text{Gd}^{3+}$ . The interaction contains the first power of orbital angular momentum  $\mathbf{l}$ , so each order of the perturbation theory in the interaction changes the selection rule by  $\Delta l = \pm 1$ . Hence, to get a nonzero octupole moment of  $\text{Gd}^{3+}$  one has to go to the second order in the spin-orbit interaction. This is a very small effect and we do not consider it.

Now we return to the energy correction (9). Expanding  $|\mathbf{r} - \mathbf{R}|^{-1}$  in a series of spherical harmonics

$$\frac{1}{|\mathbf{r} - \mathbf{R}|} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}^*(\theta_r, \phi_r) Y_{lm}(\theta_{r'}, \phi_{r'}) \quad (16)$$

where  $r_{>} = \max(r, R)$  and  $r_{<} = \min(r, R)$ ,

and keeping in mind that according to the previous discussion  $\delta\rho(\mathbf{r})$  contains only the first harmonic, we transform the energy correction (9) to the following form

$$\Delta\epsilon = e^2 \int d^3R q(\mathbf{R}) \cos\theta_R \left[ \frac{1}{R^2} \int_0^R d^3r \delta\rho(\mathbf{r}) r \cos\theta_r + R \int_R^\infty d^3r \frac{\delta\rho(\mathbf{r}) \cos\theta_r}{r^2} - \frac{1}{3R^2} \int_0^R d^3r \rho_0(\mathbf{r}) \int d^3r' \delta\rho(\mathbf{r}') r' \cos\theta'_r \right] \quad (17)$$

This formula is similar to the standard one for the Schiff moment contribution to the T,P-odd energy correction, see Refs. [17,6]. For a smooth function  $q(R)$  the eq. (17) can be easily transformed to the standard form. However the point is that in the present case the density  $q(R)$  is not a smooth function of  $R$ . Similar to the standard case, eq. (17) gives zero  $\Delta\epsilon$  if the external charge  $q(R)$  is localized outside of the  $\text{Gd}^{3+}$  core. So we have to calculate the probability for external electrons to penetrate inside the  $\text{Gd}^{3+}$  core. This calculation is performed in the following section. Considering the integral over  $\mathbf{R}$  in eq. (17), we deduce that only an asymmetric part in  $q(\mathbf{R})$  proportional to  $\cos\theta_R$  can contribute to the energy correction. There is no such term for the lattice without deformation. Hence the nonzero  $\Delta\epsilon$  is also related to the deformation of the lattice.

#### IV. PENETRATION OF OXYGEN ELECTRONS INSIDE THE $\text{GD}^{3+}$ CORE, DEFORMATION OF THE LATTICE.

In the Garnet structure any  $\text{Gd}^{3+}$  ion is surrounded by eight  $\text{O}^{2-}$  ions organized in a dodecahedron structure (slightly distorted cube) [13]. For the calculation we approximate this structure by a cube with  $\text{Gd}^{3+}$  in the middle. The Gd-O distance used is  $4.53a_B$ , where  $a_B$  is the Bohr radius. In the case of GdIG there are also uncompensated spins localized at  $\text{Fe}^{3+}$  ions. However the T,P-odd effect scales as  $Z^3$ , and therefore the contribution of Fe is negligible compared to that of Gd. An additional reason for suppression of the Fe contribution is that the crystal radius of  $\text{Fe}^{3+}$  is much smaller than that of  $\text{Gd}^{3+}$ . The quantity of interest is the charge density of external electrons  $q(\mathbf{r})$  inside the  $\text{Gd}^{3+}$  ion. The electrons are coming from the eight nearest  $\text{O}^{2-}$  ions.

The  $\text{O}^{2-}$  ion has a closed shell configuration, with 3 double occupied  $2p$ -orbitals. One can show that  $2p_\pi$  orbitals do not contribute to the effects we are interested in. So we only consider  $2p_\sigma$ -orbitals pointing towards  $\text{Gd}^{3+}$  as schematically shown in the 2-dimensional picture in Fig. 1. Hence there are 16 electrons that can potentially penetrate inside  $\text{Gd}^{3+}$ .

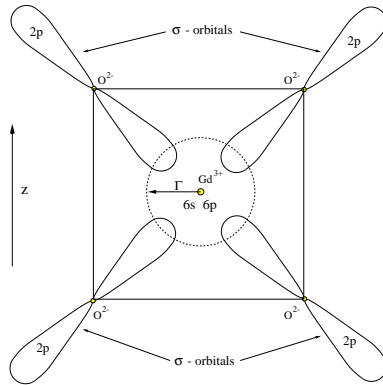


FIG. 1. A schematic 2-dimensional picture for penetration of  $2p_\sigma$ -orbitals of  $\text{O}^{2-}$  inside  $\text{Gd}^{3+}$

First of all let us rewrite the eight  $2p_\sigma$ -orbitals in the basis with definite symmetry with respect to the cubic structure. The new basis reads

$$\begin{aligned}
|S\rangle &= (1/\sqrt{8}) (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle + |7\rangle + |8\rangle) \\
|P_x\rangle &= (1/\sqrt{8}) (|1\rangle + |2\rangle - |3\rangle - |4\rangle + |5\rangle + |6\rangle - |7\rangle - |8\rangle) \\
|P_y\rangle &= (1/\sqrt{8}) (|1\rangle - |2\rangle - |3\rangle + |4\rangle + |5\rangle - |6\rangle - |7\rangle + |8\rangle) \\
|P_z\rangle &= (1/\sqrt{8}) (|1\rangle + |2\rangle + |3\rangle + |4\rangle - |5\rangle - |6\rangle - |7\rangle - |8\rangle) \\
|D_{xy}\rangle &= (1/\sqrt{8}) (|1\rangle - |2\rangle + |3\rangle - |4\rangle + |5\rangle - |6\rangle + |7\rangle - |8\rangle) \\
|D_{xz}\rangle &= (1/\sqrt{8}) (|1\rangle + |2\rangle - |3\rangle - |4\rangle - |5\rangle - |6\rangle + |7\rangle + |8\rangle) \\
|D_{yz}\rangle &= (1/\sqrt{8}) (|1\rangle - |2\rangle - |3\rangle + |4\rangle - |5\rangle + |6\rangle + |7\rangle - |8\rangle) \\
|F_{xyz}\rangle &= (1/\sqrt{8}) (|1\rangle - |2\rangle + |3\rangle - |4\rangle - |5\rangle + |6\rangle - |7\rangle + |8\rangle)
\end{aligned} \tag{18}$$

Here, for example  $|1\rangle$  denotes the  $2p_\sigma$ -orbital of the first oxygen. The ions are numbered as in Fig. 2. All of the states (18) are doubly occupied. As long as the electron is moving near the Oxygen ion the electron wave function can be described as a  $2p_\sigma$ -orbital. However when the electron approaches the  $\text{Gd}^{3+}$  ion its wave function is strongly deformed by the potential of  $\text{Gd}^{3+}$ . To describe this effect we draw an imaginary sphere of radius  $\Gamma$  around the  $\text{Gd}^{3+}$  ion as shown in Fig. 1. We assume that outside the sphere the Oxygen potential dominates and the wave is described as one of the (18) orbitals. However inside the sphere the  $\text{Gd}^{3+}$  potential dominates and hence the same orbital is described as s-, p-, d-, or f-orbital of Gd. We are interested only in s- and p- orbitals that correspond to  $|S\rangle$ ,  $|P_x\rangle$ ,  $|P_y\rangle$ , and  $|P_z\rangle$  states from (18). At  $r < \Gamma$  we will use the 6s and 6p orbitals of  $\text{Gd}^{1+}$  as the basis. We can also choose 7s and 7p or 8s and 8p, the final result is independent of the choice because at  $r < \Gamma$  all these wave functions are proportional to each other.

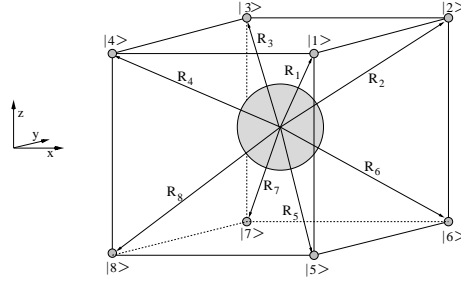


FIG. 2. The matching sphere around Gd with the surrounding eight Oxygen neighbors.

Thus at  $r < \Gamma$ , we get

$$|S\rangle \rightarrow \beta_S |6s\rangle, \quad |P_z\rangle \rightarrow \beta_P |6p_z\rangle, \quad |P_x\rangle \rightarrow \beta_P |6p_x\rangle, \quad |P_y\rangle \rightarrow \beta_P |6p_y\rangle. \tag{19}$$

To find the coefficients  $\beta_S$  and  $\beta_P$  we match (19) with (18) at the surface of the sphere with radius  $r = \Gamma$  using the following projection

$$\langle u(\Gamma, \phi, \theta) | v(\Gamma, \phi, \theta) \rangle_\Gamma = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta u^*(\Gamma, \phi, \theta) v(\Gamma, \phi, \theta). \tag{20}$$

Hence

$$\beta_S = \frac{\langle 6s | S \rangle_\Gamma}{\langle 6s | 6s \rangle_\Gamma}, \quad \beta_P = \frac{\langle 6p_z | P_z \rangle_\Gamma}{\langle 6p_z | 6p_z \rangle_\Gamma}. \tag{21}$$

This is a simple and reliable method to calculate the coefficients  $\beta_S$  and  $\beta_P$ . It has been previously used for calculation of the nuclear quadrupole resonance frequencies in  $\text{La}_2\text{CuO}_4$ , see Ref. [18]. In that case the accuracy of the method was verified by experimental data and proved to be  $\sim 10\%$ . For numerical calculations with (20),(21) we have used 2p-wave-functions of  $\text{O}^{2-}$  calculated previously in [18]. The 6s and 6p wave functions of  $\text{Gd}^{1+}$  have been obtained by the relativistic Hartree-Fock method for configuration  $1s^2 \dots 4f^7 6s 6p$ . In this calculation we average over polarizations of the unclosed shells. It means that  $4f^7$  is taken as  $4f^{14}$  with 50% population of each orbital, similarly 6s is taken as  $6s^2$  with 50% population and 6p is taken as  $6p^6$  with  $1/6=16.6\%$  population. There is also the fine structure effect: the difference between  $6p_{1/2}$  and  $6p_{3/2}$  states. However this effect is small and has been neglected in the calculation of  $\beta_P$ . The values of  $\beta_S$  and  $\beta_P$  calculated with (20),(21) for different choices of the matching radius  $\Gamma$  are presented in Table 1. The coefficients are not sensitive to the value of  $\Gamma$  and this confirms validity of the method.

| $\Gamma [a_B]$ | $\beta_S$ | $\beta_P$ | $\beta'_S$ | $\beta'_P$ | $P_s$ | $P_p$ | $\langle N_{2p} \rangle$ |
|----------------|-----------|-----------|------------|------------|-------|-------|--------------------------|
| 2.2            | -0.448    | 0.829     | 0.386      | -0.210     | 1.7%  | 2.7%  | 0.19                     |
| 2.3            | -0.446    | 0.754     | 0.345      | -0.204     | 2.1%  | 2.7%  | 0.20                     |
| 2.4            | -0.447    | 0.704     | 0.316      | -0.200     | 2.4%  | 2.7%  | 0.21                     |
| 2.5            | -0.448    | 0.650     | 0.285      | -0.196     | 3.2%  | 2.8%  | 0.23                     |
| 2.6            | -0.461    | 0.639     | 0.273      | -0.196     | 4.1%  | 3.3%  | 0.28                     |
| 2.7            | -0.478    | 0.634     | 0.263      | -0.197     | 5.0%  | 3.6%  | 0.31                     |
| 2.8            | -0.499    | 0.637     | 0.254      | -0.198     | 6.2%  | 4.5%  | 0.39                     |

TABLE I. The coefficients  $\beta_S$ ,  $\beta'_S$ ,  $\beta_P$ , and  $\beta'_P$  for expansion of Oxygen 2p-orbitals in terms of  $\text{Gd}^{1+}$  6s- and 6p-wave-functions, see eqs. (27),(19). The coefficients are presented for different values of the radius of the matching sphere  $\Gamma$ .  $P_s$  and  $P_p$  represent the probability for the corresponding Oxygen electron to penetrate inside the matching sphere.  $\langle N_{2p} \rangle$  is the average number of Oxygen 2p-electrons inside the matching sphere.

The calculation assumes that the 2p-wave-functions of  $\text{O}^{2-}$  are “rigid”, i.e. at  $r > \Gamma$  they are not influenced by Gd. This can be true only if the total probability for an Oxygen electron to penetrate inside the matching sphere,  $r < \Gamma$ , is small. To check this we calculate the probabilities

$$P_s = \beta_S^2 \int_0^\Gamma d^3r |\psi_{6s}(\mathbf{r})|^2, \quad (22)$$

$$P_p = \beta_P^2 \int_0^\Gamma d^3r |\psi_{6p}(\mathbf{r})|^2. \quad (23)$$

Numerical values of  $P_s$  and  $P_p$  are presented in Table 1, they are really very small. The average number of Oxygen electrons penetrating inside the matching sphere,

$$\langle N_{2p} \rangle = 2(P_s + 3P_p), \quad (24)$$

listed in Table 1 is also rather small. Thus, the external charge density with respect to  $\text{Gd}^{3+}$  inside the matching sphere is given by

$$q(\mathbf{r}) = q_0(\mathbf{r}) = 2\beta_S^2 |\psi_{6s}(\mathbf{r})|^2 + 2\beta_P^2 (|\psi_{6p_x}(\mathbf{r})|^2 + |\psi_{6p_y}(\mathbf{r})|^2 + |\psi_{6p_z}(\mathbf{r})|^2) \quad (25)$$

The coefficient 2 is due to the double occupancy (spin up, down) of each orbital.

It has been pointed out in the previous section that the charge density (25) is insufficient to generate a T,P-odd effect because  $q_0(\mathbf{r})$  is symmetric with respect to reflection  $\mathbf{r} \rightarrow -\mathbf{r}$ . To have an asymmetric part  $\delta q(\mathbf{r})$  one needs to consider a deformation of the lattice. We will assume that Gd is shifted along the z-axis with respect to the environment by a small displacement  $X$ , for definition of axes see Fig. 2. The displacement is shown schematically in the 2-dimensional picture in Fig. 3. In the general case the displacement can have an arbitrary direction. However we do not expect that the final answer will be very sensitive to the direction. Therefore we consider the simplest geometry: the displacement along the axis of the cube.

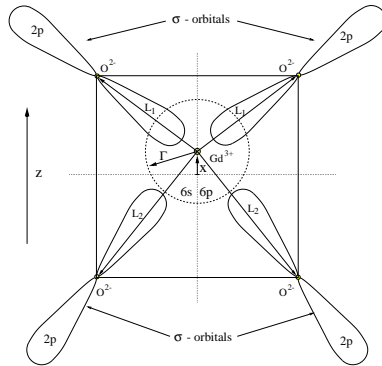


FIG. 3. A schematic 2-dimensional picture for penetration of  $2p_\sigma$ -orbitals of  $\text{O}^{2-}$  inside the shifted  $\text{Gd}^{3+}$

It is clear that outside the matching sphere nothing is changed: eqs. (18) describe the wave functions.

However inside the sphere the wave functions are changed compared to (19)

$$|S\rangle \rightarrow \beta_S |6s\rangle + \beta'_S \frac{X}{a_B} |6p_z\rangle \quad |P_z\rangle \rightarrow \beta_P |6p_z\rangle + \beta'_P \frac{X}{a_B} |6s\rangle. \quad (26)$$

We present only the orbitals that give a nonzero contribution to the T,P-odd effect. To have dimensionless coefficients  $\beta'_S$  and  $\beta'_P$  we divide the displacement by the Bohr radius. To calculate the coefficients  $\beta'_S$  and  $\beta'_P$  we use the same matching procedure (20)

$$\beta'_S = \frac{\partial}{\partial X} \frac{\langle 6p_z | S \rangle_\Gamma}{\langle 6p_z | 6p_z \rangle_\Gamma} \Big|_{X=0} \quad \beta'_P = \frac{\partial}{\partial X} \frac{\langle 6s | P_z \rangle_\Gamma}{\langle 6s | 6s \rangle_\Gamma} \Big|_{X=0} \quad (27)$$

The values of  $\beta'_S$  and  $\beta'_P$  for different values of the radius of the matching sphere  $\Gamma$  are presented in Table 1.

As one can see from Table 1 the values for  $\beta_S$ ,  $\beta_P$ ,  $\beta'_S$  and  $\beta'_P$  are almost independent of the choice  $\Gamma$  in the interval  $2.2a_B - 2.8a_B$ , this is the dual description region. Existence of this region confirms validity of our approach. For all further calculations we will use  $\Gamma = 2.5a_B$ . Using eqs. (26) we immediately obtain the asymmetric term for the charge density,

$$\delta q(\mathbf{r}) = 4(\beta_S \beta'_S + \beta_P \beta'_P) \frac{X}{a_B} \psi_{6s}(\mathbf{r}) \psi_{6p_z}(\mathbf{r}) \quad (28)$$

In the above calculation we have neglected relativistic effects. This is justified as far as the calculation of the coefficients  $\beta$  is concerned. However for the behavior of  $\delta q(\mathbf{r})$  near the Gd nucleus the relativistic effects are very important. Therefore we have to modify (28) to account for this effect. Fortunately this modification is obvious and immediately follows from decomposition of  $6p_z$  in terms of  $6p_{1/2}$  and  $6p_{3/2}$ . This gives

$$\delta q(\mathbf{r}) \rightarrow 4(\beta_S \beta'_S + \beta_P \beta'_P) \frac{X}{a_B} \left( \sqrt{\frac{2}{3}} u_s^\dagger u_{p_{3/2}} - \sqrt{\frac{1}{3}} u_s^\dagger u_{p_{1/2}} \right) \quad (29)$$

where

$$u_{p_{1/2}} = \begin{pmatrix} R_{p_{1/2}} \Omega_{p_{1/2}} \\ i \tilde{R}_{p_{1/2}} \tilde{\Omega}_{p_{1/2}} \end{pmatrix}, \quad u_{p_{3/2}} = \begin{pmatrix} R_{p_{3/2}} \Omega_{p_{3/2}} \\ i \tilde{R}_{p_{3/2}} \tilde{\Omega}_{p_{3/2}} \end{pmatrix}, \quad u_s = \begin{pmatrix} R_s \Omega_s \\ i \tilde{R}_s \tilde{\Omega}_s \end{pmatrix}, \quad (30)$$

are the Dirac wave functions of  $6p_{1/2}$ ,  $6p_{3/2}$ , and  $6s_{1/2}$  states.  $\Omega$  and  $\tilde{\Omega} = -(\boldsymbol{\sigma} \cdot \mathbf{n})\Omega$  are the usual two-component spherical spinors [19];  $R$  and  $\tilde{R}$  are upper and lower radial wave functions that have been calculated using the Relativistic Hartree-Fock method.

## V. RELATION BETWEEN THE LATTICE DEFORMATION AND THE T,P-ODD ENERGY CORRECTION INDUCED BY THE ELECTRON EDM

The T,P-odd interaction of the electron EDM with the electric field of the Gd nucleus  $\mathbf{E}$  is  $V_d = -d_e \gamma_0 \boldsymbol{\Sigma} \cdot \mathbf{E}$ , and account of the Schiff theorem for electronic degrees of freedom reduces it to the form, see e.g. Ref. [6]

$$V_d \rightarrow V_d^r = -d_e (\gamma_0 - 1) \boldsymbol{\Sigma} \cdot \mathbf{E}, \quad (31)$$

where  $\gamma_0$  and  $\boldsymbol{\Sigma} = \gamma_0 \gamma_5 \boldsymbol{\gamma}$  are Dirac  $\gamma$ -matrices. According to [14] the EDM of  $\text{Gd}^{3+}$  ion is saturated by 4f-5d mixing

$$d_a = K d_e = e \int_0^\infty d^3r \delta \rho(\mathbf{r}) r \cos \theta_r \approx 2e \sum_{m=-2}^2 \frac{\langle 4f_m | r \cos \theta_r | 5d_m \rangle \langle 5d_m | V_d^r | 4f_m \rangle}{E_{4f} - E_{5d}}. \quad (32)$$

Diagrammatically it is shown in Fig. 4

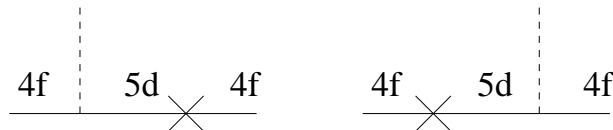


FIG. 4. Leading contribution to  $\text{Gd}^{3+}$  EDM. The dashed line denotes the dipole moment  $ez = er \cos \theta$ , and the cross denotes the T,P-odd interaction  $V_d^r$ , eq (31).

The same 4f-5d virtual transitions saturate the T,P-odd correction to energy (17), and taking into account eq. (29) the correction (17) can be rewritten as

$$\begin{aligned}\Delta\epsilon &= \frac{4e^2}{\sqrt{3}}(\beta_S\beta'_S + \beta_P\beta'_P) \frac{X}{a_B} 2 \sum_{m=-3}^3 \frac{\langle Y_{3m} | \cos\theta | Y_{4m} \rangle \langle 5d_m | V_d^r | 4f_m \rangle}{E_{4f} - E_{5d}} (I_1 + I_2 + I_3) \\ &= \frac{4e}{\sqrt{3}}(\beta_S\beta'_S + \beta_P\beta'_P) \frac{X}{a_B} \frac{K d_e}{\langle r_{fd} \rangle} (I_1 + I_2 + I_3).\end{aligned}\quad (33)$$

where,

$$\begin{aligned}I_1 &= \int_0^\Gamma dR \left( \frac{1}{3}(R_s R_{p_{1/2}} + \tilde{R}_s \tilde{R}_{p_{1/2}}) + \frac{2}{3}(R_s R_{p_{3/2}} + \tilde{R}_s \tilde{R}_{p_{3/2}}) \right) \int_0^R dr r^3 R_{4f}(r) R_{5d}(r), \\ I_2 &= \int_0^\Gamma dR R^3 \left( \frac{1}{3}(R_s R_{p_{1/2}} + \tilde{R}_s \tilde{R}_{p_{1/2}}) + \frac{2}{3}(R_s R_{p_{3/2}} + \tilde{R}_s \tilde{R}_{p_{3/2}}) \right) \int_R^\Gamma dr R_{4f}(r) R_{5d}(r), \\ I_3 &= -\frac{1}{3} \int_0^\Gamma dR \left( \frac{1}{3}(R_s R_{p_{1/2}} + \tilde{R}_s \tilde{R}_{p_{1/2}}) + \frac{2}{3}(R_s R_{p_{3/2}} + \tilde{R}_s \tilde{R}_{p_{3/2}}) \right) \int_0^R d^3r \rho_0(\mathbf{r}) \int_0^\Gamma dr' r'^3 R_{4f}(r') R_{5d}(r'), \\ \langle r_{fd} \rangle &= \int_0^\Gamma dr' r'^3 R_{4f}(r') R_{5d}(r'),\end{aligned}\quad (34)$$

In the integrals we have replaced the upper limit of integration by  $\Gamma = 2.5a_B$ , because eq. (29) is valid only at  $r < \Gamma$ . The final result is not sensitive to the upper limit because these integrals are convergent at smaller distances. The numerical values obtained with Hartree-Fock wave functions are

$$I_1 = -4.1 \times 10^{-3} a_B^{-1}, \quad I_2 = -5.3 \times 10^{-3} a_B^{-1}, \quad I_3 = -7.5 \times 10^{-3} a_B^{-1}, \quad \langle r_{fd} \rangle = 0.55a_B. \quad (35)$$

Substituting these values, as well as the value of the coefficient  $K$  from (3) and the coefficients  $\beta$  from Table 1. in eq. (33) we find the T,P-odd energy correction per Gd ion as a function of the ion displacement with respect to surrounding Oxygen ions.

$$\Delta\epsilon(X) = -A \frac{e}{a_B^2} \frac{X}{a_B} d_e \rightarrow -A \frac{e}{S} \frac{d_e}{a_B^3} (\mathbf{X} \cdot \mathbf{S}) \quad \text{with } A = 0.11. \quad (36)$$

The vector form is valid for an arbitrary direction of the displacement  $\mathbf{X}$  and an arbitrary direction of the  $\text{Gd}^{3+}$  polarization  $\mathbf{S}/S$ . The integrals (35) give  $A = 0.09$ , however they only account for the contribution of 2p-orbitals of Oxygen. We know [18] that there is also a contribution of 2s-orbitals of Oxygen that is 20%-25% of the 2p-contribution. This is why we take  $A = 0.11$ .

The integral  $I_3$  corresponds to the compensating term in (17) and the contributions corresponding to the integrals  $I_1$  and  $I_2$  can be represented diagrammatically as shown in Fig.5

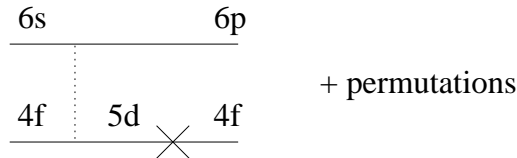


FIG. 5. Direct contribution to the T,P-odd energy shift. The dotted line denotes the Coulomb electron-electron interaction, and the cross denotes the T,P-odd interaction  $V_d^r$ , eq (31).

This is what we have taken into account and these are direct diagrams only. In principle there are also exchange diagrams shown schematically in Fig. 6 that we have neglected.

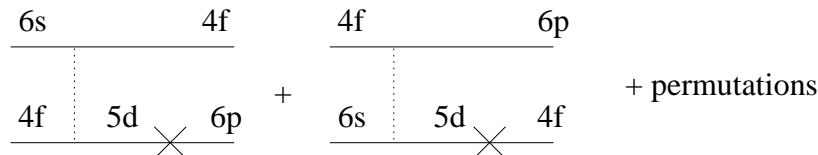


FIG. 6. Exchange contribution to the T,P-odd energy shift. The dotted line denotes the Coulomb electron-electron interaction, and the cross denotes the T,P-odd interaction  $V_d^r$ , eq (31).



The exchange diagrams have higher angular momenta of the Coulomb quantum than the direct ones, the diagrams in Fig.6 have  $k = 2, 3, 4$ , while the direct diagram in Fig.5 has  $k = 1$ . Therefore it is unlikely that the exchange contributions can be comparable with direct ones. Nevertheless, at some later stage, these contributions have to be calculated as well.

## VI. T,P-ODD VOLTAGE ACROSS A MAGNETICALLY POLARIZED SAMPLE OF GDIG

In this section we consider a GdIG sample magnetically polarized along some axis. Then according to eq. (36) each Gd ion can gain energy from a small distortion of the lattice. However the lattice has stiffness and therefore the total variation of energy per Gd ion as a function of the displacement  $X$  is of the form

$$\Delta\epsilon_T = \frac{1}{2}K_{el}X^2 - A\frac{e}{a_B^2}\frac{X}{a_B}d_e, \quad (37)$$

where  $K_{el}$  is the effective elastic constant per Gd ion. Minimizing (37) with respect to the lattice deformation  $X$  we find the deformation induced by the electron EDM.

$$X = \frac{Ae}{K_{el}a_B^3}d_e. \quad (38)$$

To calculate the deformation we need to know the value of  $K_{el}$ . The elastic constant is related to optic phonons, and can be found from the spectra of the phonons. However we will use a simpler method based on the known static dielectric constant of GdIG,  $\epsilon \approx 15$  [16]. Consider some external electric field applied to the GdIG sample. According to standard relations

$$\mathbf{D} = \epsilon\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}, \quad (39)$$

where  $\mathbf{E}$  is the average electric field in the sample and  $\mathbf{P}$  the polarization per unit volume. Assuming simple cubic structure the local field acting on each ion is [20]

$$\mathbf{E}_l = \mathbf{E} + \frac{4\pi}{3}\mathbf{P} = 4\pi\mathbf{P}\left(\frac{1}{\epsilon-1} + \frac{1}{3}\right) \quad (40)$$

This gives the displacement of the  $\text{Gd}^{3+}$  ion in the field

$$x_1 = \frac{3eE_l}{K_{el}} = \frac{12\pi e}{K_{el}}P\left(\frac{1}{\epsilon-1} + \frac{1}{3}\right) \quad (41)$$

Similarly one can find the displacement of the  $\text{Fe}^{3+}$  ion  $x_2$  in terms of the corresponding elastic constant  $K'_{el}$ . On the other hand, the polarization per unit volume by definition is  $P = 3ex_1n_{Gd} + 5ex_2n_{Gd}$ . Altogether this gives the following result for  $K_{el}$ .

$$K_{el} = 96\pi e^2n_{Gd}\left(\frac{1}{\epsilon-1} + \frac{1}{3}\right)\left(\frac{3}{8} + \frac{5K_{el}}{8K'_{el}}\right). \quad (42)$$

We recall that  $n_{Gd} = 1.235 \times 10^{22} \text{ cm}^{-3}$  is the number density of Gd in GdIG. For further estimates we will assume that  $K_{el} = K'_{el}$ . There is no reason for these constants to differ substantially, and moreover eq. (42) is not that sensitive to the ratio  $K_{el}/K'_{el}$ .

Coming back to the situation without any external electric field and using eqs. (38) and (42) we find the electric polarization  $P = 3eXn_{Gd}$  and hence the electric field inside the sample

$$E = -4\pi P = -\frac{A}{8\left(\frac{1}{\epsilon-1} + \frac{1}{3}\right)} \cdot \frac{d_e}{a_B^3} = -0.54 \times 10^{-10} \text{ V/cm}. \quad (43)$$

This numerical value corresponds to the current upper limit on the electron EDM (1). For a 10 cm sample it gives a voltage  $\Delta V = 0.54 \times 10^{-9} \text{ V}$ . This is smaller than the naive estimate (4) and this is suppression due to the Schiff theorem. Fortunately this suppression is not strong.

## VII. T,P-ODD MAGNETIZATION OF GGG IN THE EXTERNAL ELECTRIC FIELD

Following the suggestion of Lamoreaux [1] we consider now a different kind of experiment: an external electric field is applied to the sample and this leads to the macroscopic magnetization. Equation (41) gives the Gd shift due to the electric field.

$$X = \frac{(\epsilon - 1)}{32\pi en_{Gd}} E \quad (44)$$

Substituting this into eq. (36) we find the energy shift of the  $\text{Gd}^{3+}$  ion

$$\Delta\epsilon = -\frac{A(\epsilon - 1)}{32\pi(a_B^3 n_{Gd})} d_e \frac{(\mathbf{E} \cdot \mathbf{S})}{S} \rightarrow 2.8 \times 10^{-22} eV. \quad (45)$$

The numerical estimate corresponds to  $E = 10 \text{ kV/cm}$ , the current limitation on  $d_e$ , (1), and the dielectric constant  $\epsilon \approx 30$  for GGG [16]. It is interesting that in spite of the Schiff theorem the result (45) is larger than the naive estimate (5).

The energy shift (45) leads to the macroscopic magnetization of the sample. The magnetization depends also on temperature and internal magnetic interactions in the compound. We do not discuss these points here. According to estimates [1] the magnetization due to the energy shift  $\sim 10^{-22} eV$  can be measured and moreover the prospects for improvement of sensitivity are very good.

## VIII. T,P-ODD VOLTAGE AND MAGNETIZATION DUE TO THE NUCLEAR SCHIFF MOMENT

The effects considered above are due to the electron EDM, so they are sensitive to T,P-violation in the lepton sector. Similar effects are generated by the Nuclear Schiff Moment (NSM), so they are also sensitive to T,P-violation in the hadron sector. We begin from consideration of the same compounds GdIG and GGG, assuming only one Gd isotope. This must be an odd isotope, say  $^{155}\text{Gd}$ . The NSM  $\mathbf{S}_N$  is a T,P-odd vector moment that is a property of the nucleus, see Refs. [17,6]

$$\mathbf{S}_N = S_N \frac{\mathbf{I}}{I}, \quad (46)$$

where  $\mathbf{I}$  is nuclear spin. In previous sections we denoted by  $\mathbf{S}$  the total electron spin, note that it has nothing in common with the NSM  $\mathbf{S}_N$ . Due to the Schiff moment there is the T,P-odd interaction between electron and nucleus. This is the contact interaction, therefore the matrix elements of the interaction are nonzero only for s- and p-electrons. These matrix elements have been calculated in Ref. [17], see also [6]

$$\langle s | H_S | p \rangle = \frac{Z^2 e R}{\pi a_B^4 (\nu_s \nu_p)^{3/2}} \mathbf{S}_N \langle \Omega_s | \mathbf{n} | \Omega_p \rangle. \quad (47)$$

Here  $\Omega_s$  and  $\Omega_p$  are spherical spinors corresponding to the s- and p-states;  $\mathbf{n}$  is the unit vector;  $\nu_s$  and  $\nu_p$  are principal effective quantum numbers; and  $R$  is the relativistic factor that is different for  $p_{1/2}$  and  $p_{3/2}$  electrons

$$R_{1/2} \approx \frac{4\gamma_{1/2} x_0^{2\gamma_{1/2}-2}}{[\Gamma(2\gamma_{1/2} + 1)]^2}, \quad (48)$$

$$R_{3/2} \approx \frac{48\gamma_{1/2} x_0^{\gamma_{1/2}+\gamma_{3/2}-3}}{\Gamma(2\gamma_{1/2} + 1)\Gamma(2\gamma_{3/2} + 1)}.$$

Here  $\gamma_{1/2} = \sqrt{1 - Z^2 \alpha^2}$ ,  $\gamma_{3/2} = \sqrt{4 - Z^2 \alpha^2}$ ,  $\alpha$  is the fine structure constant;  $\Gamma(x)$  is the usual  $\gamma$ -function; and  $x_0 = (2Zr_0/a_B)$ , where  $r_0$  is the nuclear radius. For Gd,  $R_{1/2} = 3.56$  and  $R_{3/2} = 2.99$ . Assuming that the nucleus is completely polarized along the z-axis, and taking also  $|p\rangle \rightarrow |p_z\rangle$  we find from (47)

$$\langle s | H_S | p_z \rangle = \frac{S_N Z^2 e}{\pi \sqrt{3} a_B^4 (\nu_s \nu_p)^{3/2}} \left( \frac{1}{3} R_{1/2} + \frac{2}{3} R_{3/2} \right) \quad (49)$$

According to (26) lattice deformation  $X$  leads to the mixing of 6s- and 6p-orbitals. Hence the matrix element of  $H_S$  over the electronic states of the deformed lattice is equal to

$$\langle H_S \rangle = \frac{4}{\pi \sqrt{3}} (\beta_S \beta'_S + \beta_P \beta'_P) \frac{X}{a_B} \frac{S_N Z^2 e}{a_B^4 (\nu_s \nu_p)^{3/2}} \left( \frac{1}{3} R_{1/2} + \frac{2}{3} R_{3/2} \right). \quad (50)$$

The effective principal numbers for 6s- and 6p-orbitals are:  $\nu_{6s} = 1.24$ ,  $\nu_{6p_{1/2}} = 1.46$ , and  $\nu_{6p_{3/2}} = 1.49$ , see comment [21]. Substituting these values, together with coefficients  $\beta$  from Table 1 and all the other parameters we find the T,P-odd energy correction due to the NSM

$$\Delta\epsilon(X) = -B \frac{e}{a_B^4} \frac{X}{a_B} S_N \rightarrow -B \frac{e}{I} \frac{S_N}{a_B^5} (\mathbf{X} \cdot \mathbf{I}) \quad \text{with} \quad B = 1.2 \times 10^3. \quad (51)$$

The vector form is valid for an arbitrary direction of the displacement  $\mathbf{X}$  and an arbitrary direction of the Gd nuclear spin  $\mathbf{I}$ . Equation (51) for the energy shift due to NSM is similar to eq. (36) for the energy shift due to the electron EDM. We stress once more that  $S_N$  in (51) denotes the NSM while  $S$  in (36) denotes the electron spin. In (51) we have also taken into account 20% contribution from the Oxygen 2s-electrons, see comment after eq. (36).

Next we follow the same path as we did for the effects due to the electron EDM. First consider a sample with fully polarized nuclear spins, no external electric field. Then, repeating the calculations performed in Section VI we find the following electric field induced inside the solid

$$E = -\frac{B}{8 \left( \frac{1}{\epsilon-1} + \frac{1}{3} \right)} \cdot \frac{S_N}{a_B^5} = -0.9 \times 10^{-12} \text{V/cm}. \quad (52)$$

The numerical value corresponds to the current upper limit on the NSM of  $^{199}\text{Hg}$  (2).

If the external electric field is applied to the solid then repeating the calculations from Section VII we find the energy shift per Gd depending on the orientation of Gd nucleus

$$\Delta\epsilon = -\frac{B(\epsilon-1)}{32\pi(a_B^3 n_{Gd})} \cdot \frac{S}{a_B^2} \cdot \frac{(\mathbf{E} \cdot \mathbf{I})}{I} \rightarrow -0.47 \times 10^{-23} \text{eV}. \quad (53)$$

The numerical estimate corresponds to  $E = 10 \text{kV/cm}$ , the current limitation on NSM of  $^{199}\text{Hg}$  (2), and the dielectric constant  $\epsilon \approx 30$  for GGG [16].

## IX. ACCURACY OF THE CALCULATIONS

The effects related to the Nuclear Schiff moment are sensitive only to s- and p-orbitals of Gd. There are three sources of possible corrections to the results presented in eqs. (51), (52), and (53): 1)interatomic many-body correlations, 2)inaccuracy of the used matching procedure for calculation of the expansion coefficients  $\beta$ , 3)deviation of the effective elastic constant  $K_{el}$  for Gd from that for Fe. Usually for s- and p-orbitals the correction due to the interatomic correlations does not exceed 20%, see e.g. [6]. As we already mentioned above the matching procedure has been previously used for calculation of the nuclear quadrupole resonance frequencies in  $\text{La}_2\text{CuO}_4$ , see Ref. [18]. In that case the accuracy of the procedure was verified by experimental data and proved to be about 10%. We believe that this estimate is also valid for the present case. Finally, even in the unlikely case of 40% difference in elastic constants  $K_{el}$  and  $K'_{el}$  the variation in (52) and (53) is 20%. All in all this gives a 20%-30% estimate for a possible inaccuracy in (51), (52), and (53).

Situation with effects induced by the electron EDM is more complex. The mechanisms 1-3 for possible corrections contribute here as well. The interatomic many-body correlations have been considered in Ref. [14]. They contribute at the level 20%, but the most important ones have already been accounted in the value of the EDM enhancement coefficient  $K$  we used in the present work. In addition there are uncertainties due to 4)experimentally unknown  $E_{4f} - E_{5d}$  energy splitting in  $\text{Gd}^{3+}$ , and 5)unaccounted exchange diagrams in Fig.6. The most important is the energy splitting  $E_{4f} - E_{5d}$  that determines uncertainty in the electron EDM enhancement coefficient  $K$ , see eq.(3). We estimate the accuracy of the results (36), (43), and (45) as 30-40%. Experimental and/or theoretical determination of the  $E_{4f} - E_{5d}$  energy splitting in  $\text{Gd}^{3+}$  would be the most important to improve the accuracy of the calculation of the effects related to the electron EDM.

## X. CONCLUSIONS

In the present work we have considered the T,P-odd effects in solids. The calculations are performed for Gadolinium Gallium Garnet,  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  (GGG), and Gadolinium Iron Garnet  $\text{Gd}_3\text{Fe}_5\text{O}_{12}$  (GdIG). We consider the effects due to the electron electric dipole moment (EDM) and due to the Nuclear Schiff Moment (NSM). Both GdIG and GGG have uncompensated electron spins on  $\text{Gd}^{3+}$  ions. There are two possibilities to probe the electron EDM. The first one is to polarize magnetically the electron spins and to measure the induced voltage across the sample. According to our calculations at the current limitation on the electron EDM, (1), the induced

voltage across a 10cm sample is  $0.54 \times 10^{-9}V$ , see eq. (43). Another possibility is to apply an electric field to the unpolarized sample. This leads to the spin-dependent energy shift of each Gd ion  $\Delta\epsilon = 2.8 \times 10^{-22}eV$  at  $E = 10kV/cm$ , see eq. (45). This can be measured via macroscopic magnetization of the sample.

Gd nuclei can be polarized by the electron polarization via the hyperfine interaction or they can be polarized independently. For 100% polarization at the current limitation on the NSM (2) the induced voltage across a 10cm sample is  $0.9 \times 10^{-11}V$ , see eq. (52). Application of the external electric field to the unpolarized sample leads to the energy shift of each Gd  $\Delta\epsilon = 0.47 \times 10^{-23}eV$  at  $E = 10kV/cm$ , see eq. (53). The shift is dependent on the nuclear spin. This can be measured in NMR experiments or via macroscopic electronic magnetization of the sample due to the hyperfine interaction.

Another possibility for searches of NSM is to use compounds without unpaired electrons, such as Lutetium Gallium Garnet,  $Lu_3Ga_5O_{12}$  or Lutetium Oxide  $Lu_2O_3$ . In this case both the NMR and the macroscopic magnetization techniques can be used. A possibility to cool the nuclear spin subsystem down to very low temperatures [12] can give an additional advantage.

In our estimates of the effects induced by NSM we have used the current limitation (2) for NSM of  $^{199}Hg$  as the reference point. However the NSM is dependent on nucleus.  $^{199}Hg$  is a simple spherical nucleus while  $^{155}Gd$  is a deformed nucleus with close (105keV) levels of opposite parity and low energy ( $\sim 1MeV$ ) collective  $3^-$  excitation. In this situation an additional enhancement of NSM by an order of magnitude is possible. This problem requires separate consideration.

There is one more mechanism to probe T,P-violation inside nucleus. It is related to the T,P-odd nuclear electric octupole moment and it also requires separate consideration. This mechanism was mentioned in Ref [17], but has never been considered. For  $^{155}Gd$  it can give a large contribution because of the low energy collective  $3^-$  excitation.

## ACKNOWLEDGMENTS

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